

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF103118\
 Data File : BF110335.D
 Acq On : 31 Oct 2018 16:20
 Operator : JU/SJ
 Sample : J5202-15 2X
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PL-03-103018-B

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102318.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.251	24	28	39	rVB	109859	172973	23.52%	2.186%
2	5.198	525	529	534	rBV	20119	25167	3.42%	0.318%
3	5.592	592	596	609	rBV	661955	656215	89.23%	8.294%
4	6.592	762	766	786	rBV	675076	680798	92.57%	8.605%
5	6.739	788	791	799	rBV	769854	682329	92.78%	8.624%
6	6.975	828	831	837	rBV	460422	378954	51.53%	4.790%
7	7.128	854	857	866	rBV	616864	527402	71.71%	6.666%
8	7.533	922	926	938	rBV	364962	372438	50.64%	4.707%
9	8.257	1046	1049	1054	rBV	423439	401506	54.60%	5.075%
10	9.327	1228	1231	1253	rVB	674454	675711	91.88%	8.540%
11	9.722	1295	1298	1305	rBV	62108	61904	8.42%	0.782%
12	10.016	1345	1348	1362	rBV	429619	467118	63.52%	5.904%
13	10.810	1480	1483	1496	rBV	363766	393028	53.44%	4.968%
14	11.516	1599	1603	1612	rBV	536233	494072	67.18%	6.245%
15	12.016	1684	1688	1691	rBV2	7139	9478	1.29%	0.120%
16	12.739	1808	1811	1813	rBV	15383	15435	2.10%	0.195%
17	12.968	1848	1850	1853	rVB	16376	15787	2.15%	0.200%
18	13.098	1868	1872	1875	rBV	897533	735415	100.00%	9.295%
19	13.980	2019	2022	2026	rBV2	50655	64362	8.75%	0.813%
20	14.168	2050	2054	2060	rBV	531730	525181	71.41%	6.638%
21	15.286	2241	2244	2254	rVB	95837	154677	21.03%	1.955%
22	15.709	2314	2316	2322	rVB2	228464	279311	37.98%	3.530%
23	16.151	2388	2391	2397	rVB	87925	122721	16.69%	1.551%

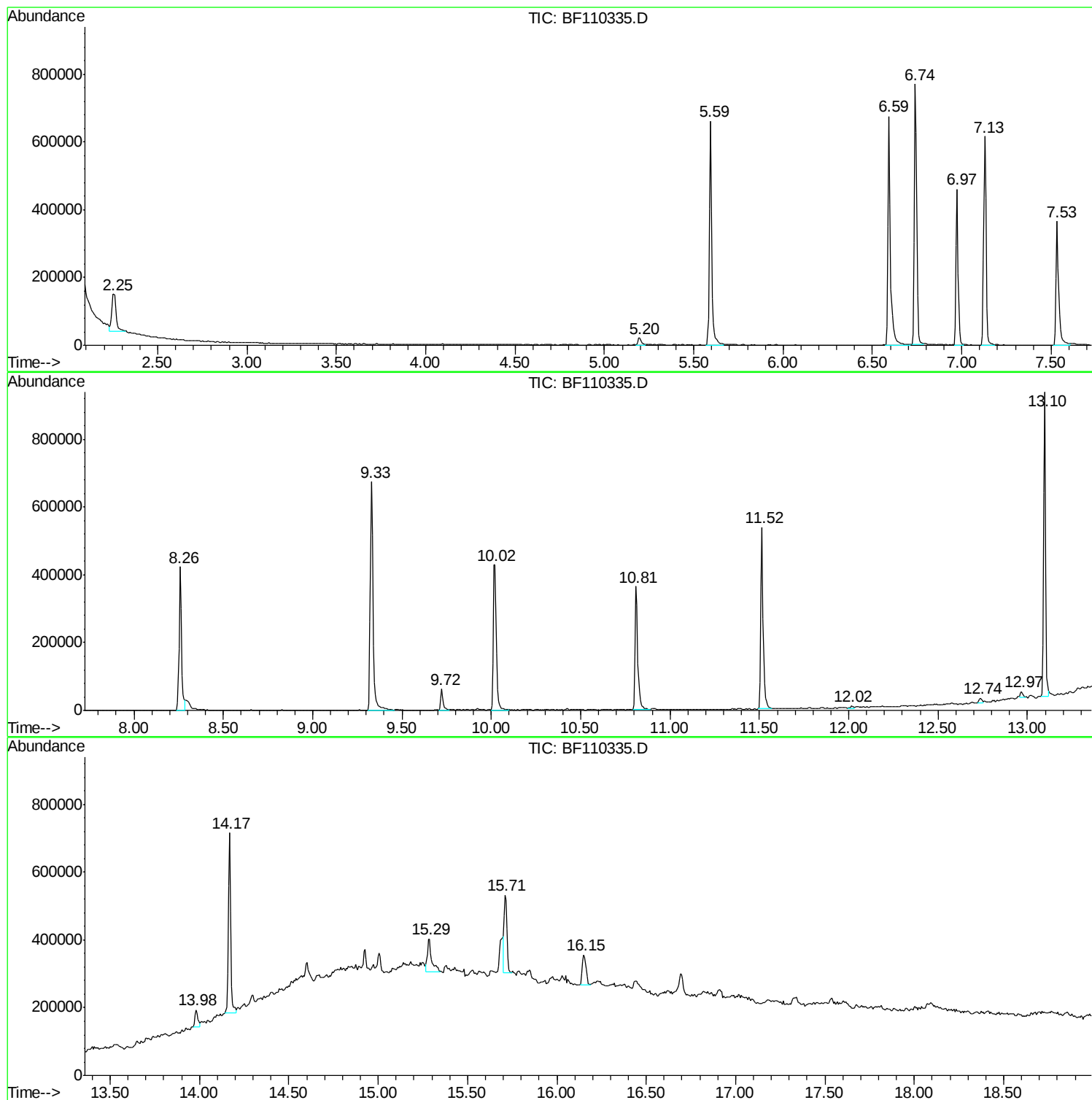
Sum of corrected areas: 7911982

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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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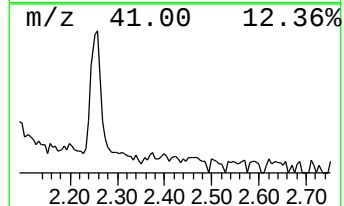
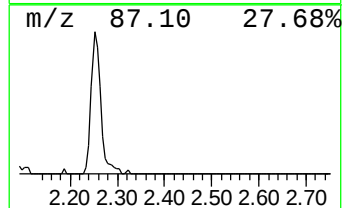
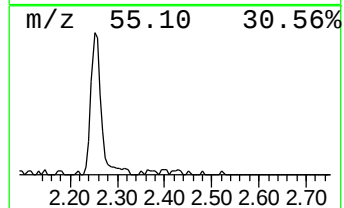
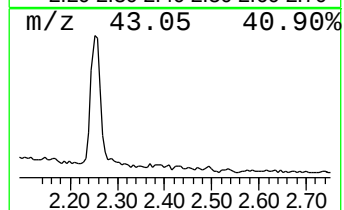
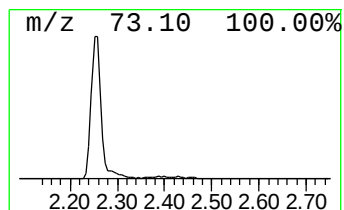
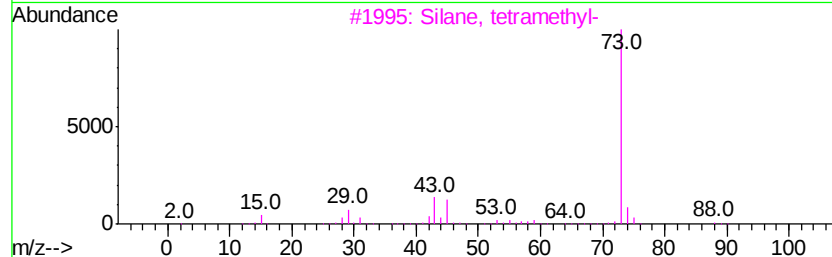
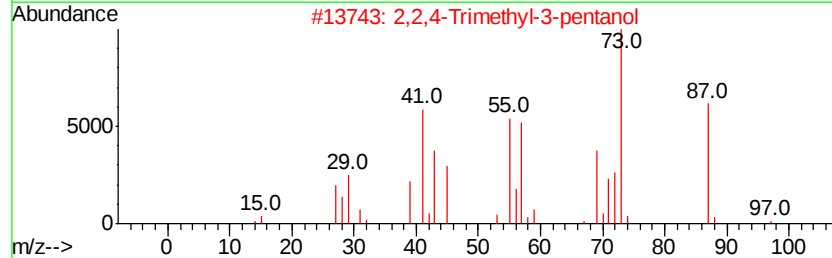
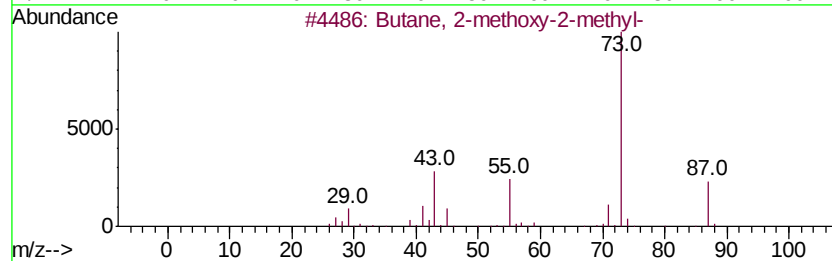
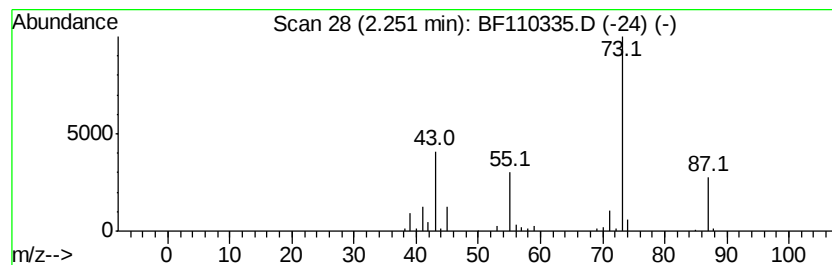
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF102318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	9.13 ng	172973	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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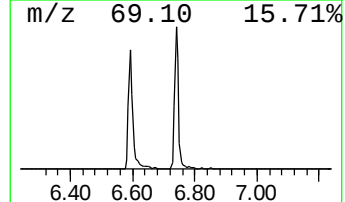
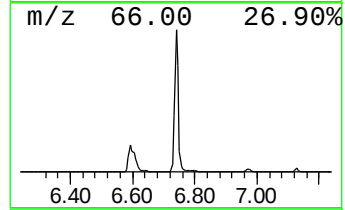
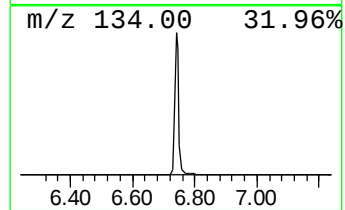
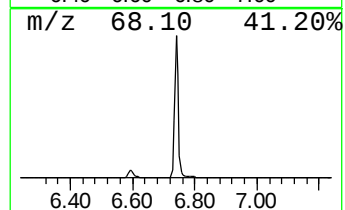
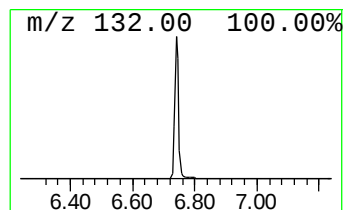
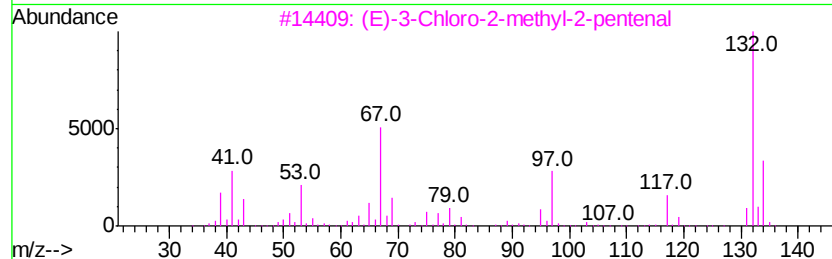
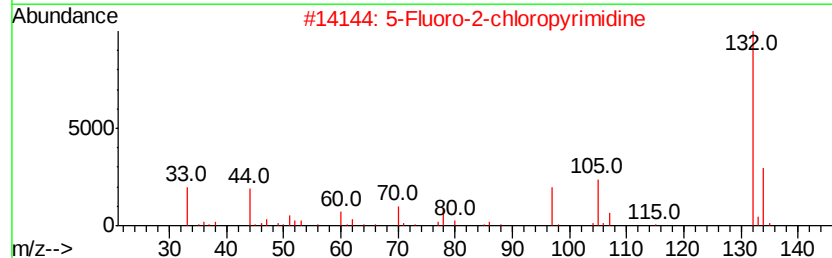
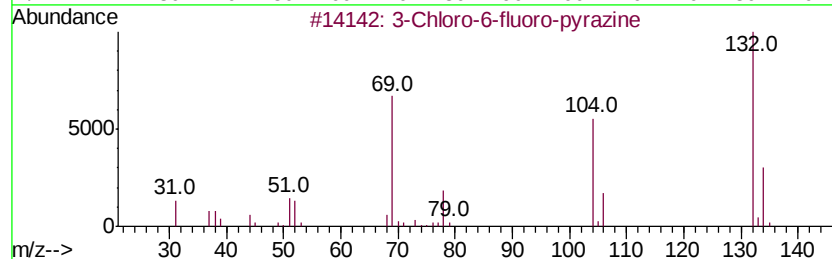
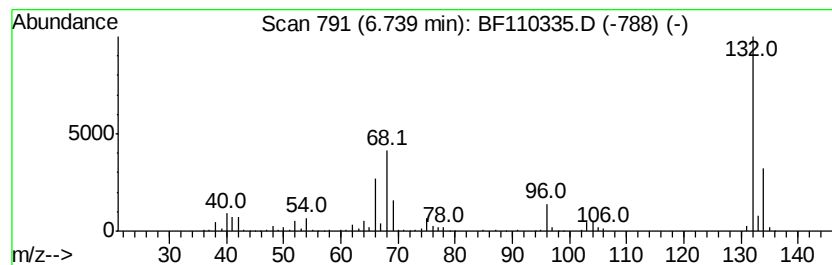
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	36.01 ng	682329	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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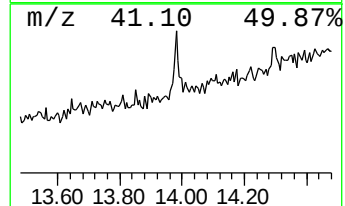
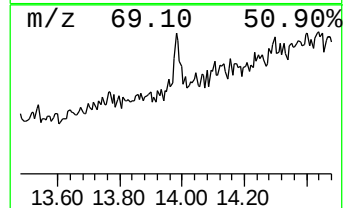
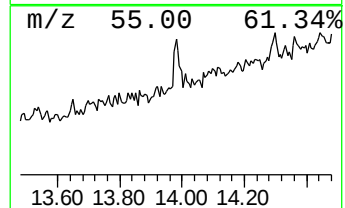
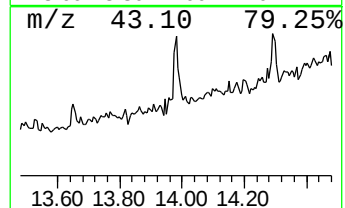
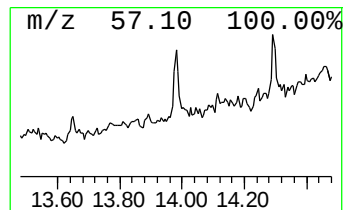
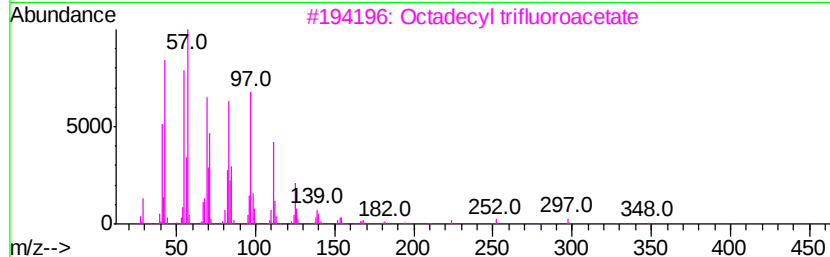
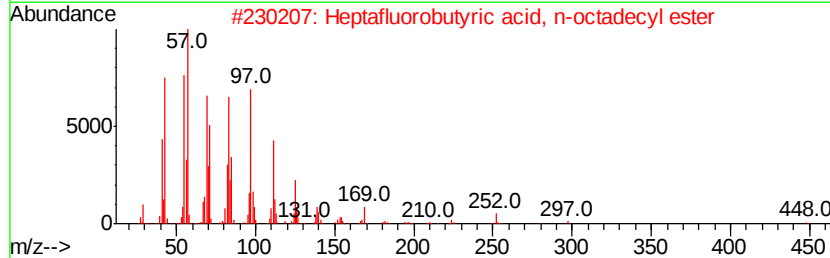
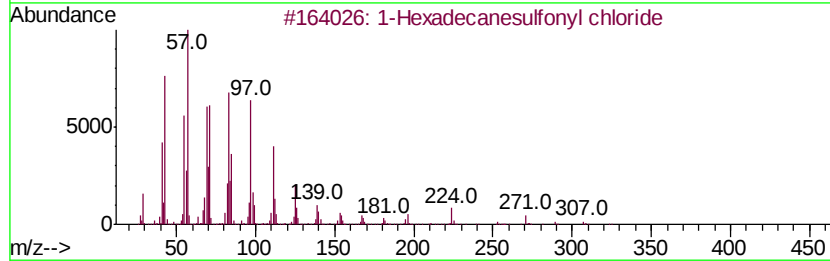
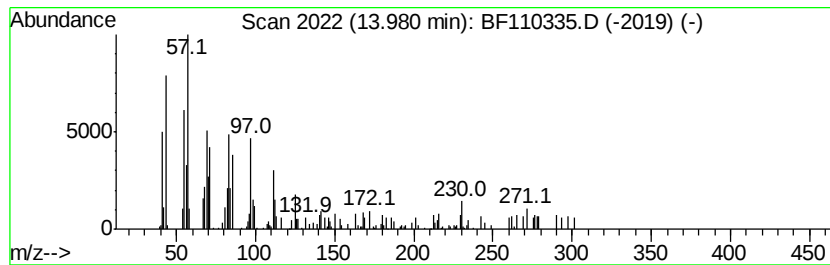
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Peak Number 4 1-Hexadecanesulfonyl chloride Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.98	2.45 ng	64362	Chrysene-d12		14.17	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Hexadecanesulfonyl chloride	324	C16H33ClO2S	038775-38-1	83
2		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	83
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	83
4		Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	83
5		Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	74



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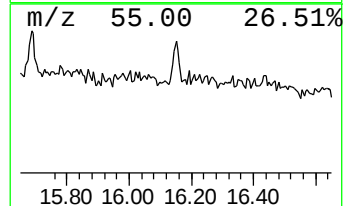
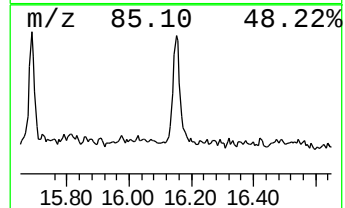
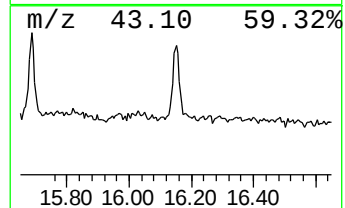
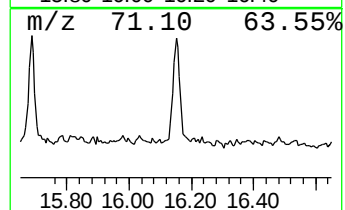
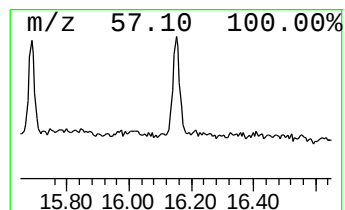
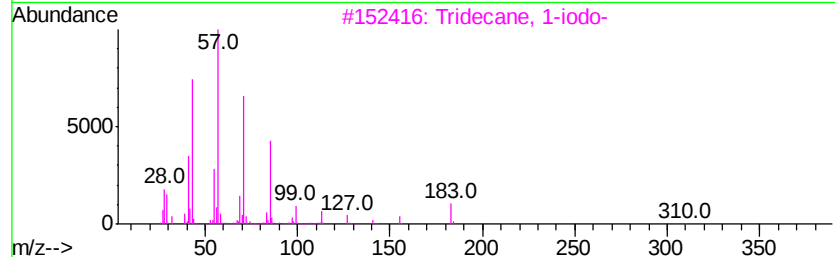
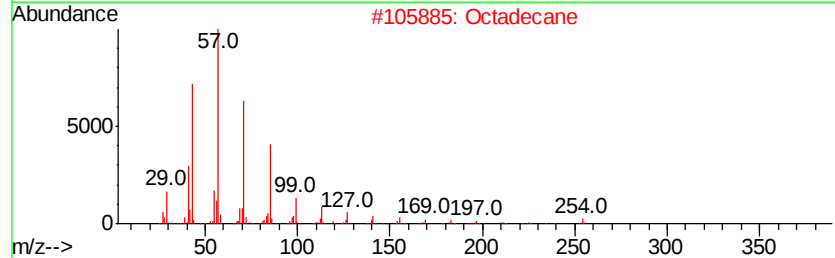
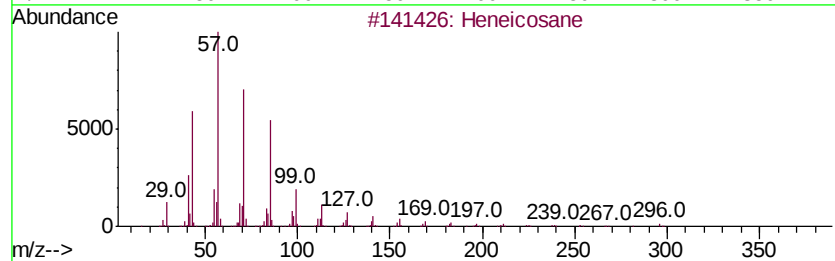
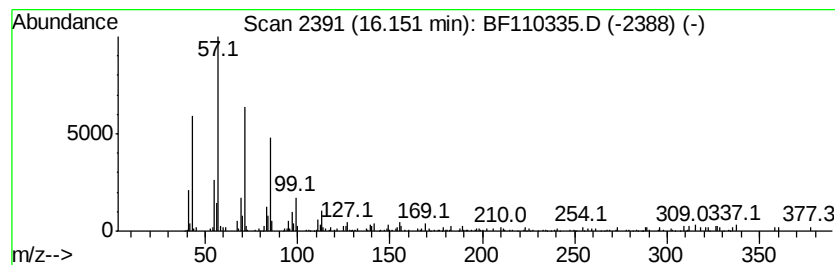
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Peak Number 6 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.15	8.79 ng	122721	Perylene-d12	15.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane		296	C21H44	000629-94-7	97
2	Octadecane		254	C18H38	000593-45-3	92
3	Tridecane, 1-iodo-		310	C13H27I	035599-77-0	91
4	Docosane		310	C22H46	000629-97-0	90
5	Hentriacontane		437	C31H64	000630-04-6	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.25	9.1	ng	172973	1	6.97	378954	20.0
unknown6.74	6.74	36.0	ng	682329	1	6.97	378954	20.0
1-Hexadecanesulfo...	13.98	2.5	ng	64362	5	14.17	525181	20.0
Heneicosane	16.15	8.8	ng	122721	6	15.71	279311	20.0